Sulfurous acid, bis(2-methylpropyl) ester

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -1.89 °C

Global applicability domain: Inside

Local applicability domain index: 5.31e-01

Confidence level: 4.93e-01

Nearest Neighbors from the Training Set

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Diethyl sulfate
Measured: -24.0
Predicted: -14.8

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Propanedioic acid, oxo-, diethyl
ester
Measured: -30.0
Predicted: 1.01e-01

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Ethyl 2,4-dioxovalerate
Measured: 18.0
Predicted: 27.4

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1,4-Dioxacyclohexadecane-5,16-
dione
Measured: 18.0
Predicted: 35.5